

Statistical and Low Temperature Physics (PHYS393)

2. Electrons in metals

Kai Hock

2010 - 2011

University of Liverpool

Contents

2.1 Fermi-Dirac statistics

2.2 Electronic heat capacity

2.3 Effective mass, and a few other things

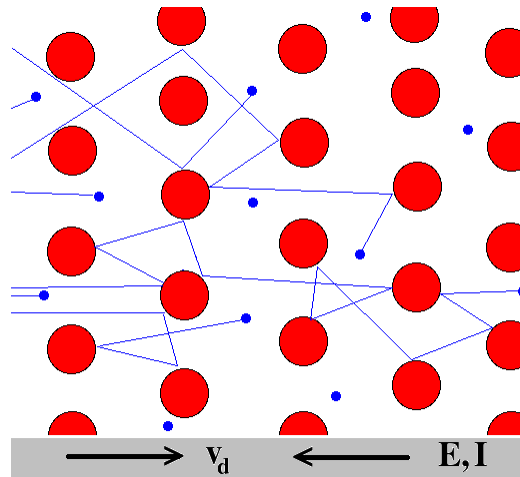
2.4 Exercises

2.1 Fermi-Dirac statistics

Electrons in a metal

The Drude model was proposed in 1900 by Paul Drude to explain the transport properties of electrons in a metal.

This treats the electrons like an ideal gas.



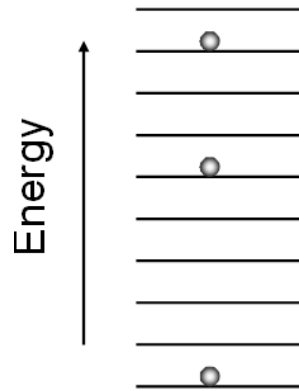
It explains very well the DC and AC conductivity in metals, the Hall effect, and thermal conductivity.

However, it greatly overestimates the heat capacities.

http://en.wikipedia.org/wiki/Drude_model

Why did the electron gas model fail?

When we derived the Maxwell-Boltzmann distribution for the ideal gas, we assumed that it is extremely unlikely for two atoms to occupy the same energy level.



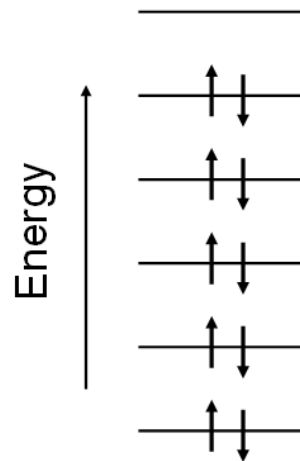
The reason is that the energy levels are very close together, compared to the average energy of the atoms.

Unfortunately, this is no longer true for electrons in a metal at room temperature. (Prove it.)

The exclusion principle

Electrons are not allowed to occupy the same energy states.

So they have to be stacked up from bottom to top.



When heated, most of the electrons are stuck - there is no space above to move up in energy !

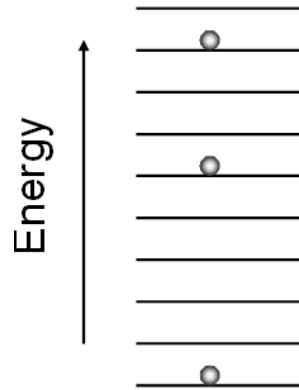
Only those few at the very top can. As a result, the heat capacities are much smaller than expected of a gas.

Fermi-Dirac statistics

As a result, we cannot use the Maxwell-Boltzmann distribution for the ideal gas.

Fortunately, we can use the same statistical methods that we have learnt so far.

Lets start by looking at the states in an energy interval $d\varepsilon$.



We have g_i energy states in the interval. Suppose the interval contains n_i electrons.

Fermi-Dirac distribution

According to the exclusion principle, exactly n_i states must be filled and exactly $g_i - n_i$ states unfilled.

The total number of ways the electrons can be arranged in this bundle is therefore:

$$\Omega_i = \frac{g_i!}{n_i!(g_i - n_i)!}$$

For the whole system - i.e. all the bundles - we get

$$\Omega = \prod_i \frac{g_i!}{n_i!(g_i - n_i)!}$$

Applying the Lagrange multiplier method again, we would get

$$\frac{n_i}{g_i} = \frac{1}{\exp(-\lambda_1 - \lambda_2 \varepsilon_i) + 1}$$

where λ_1 and λ_2 are the Lagrange multipliers.

We have applied the same constraints as before on the particle number N and the energy U .

Previously, we have used $n(\varepsilon)$ for the number density, $g(\varepsilon)$ for density of states, and $d\varepsilon$ for the energy interval of the bundle.

We also know that one of the Lagrange multipliers would be related to temperature:

$$\lambda_2 = -1/k_B T$$

The distribution of the electrons may then be written as

$$n(\varepsilon)d\varepsilon = \frac{g(\varepsilon)d\varepsilon}{\exp(-\lambda_1 + \varepsilon/k_B T) + 1}.$$

This is called the Fermi-Dirac distribution function.

We have obtained the Fermi-Dirac distribution function.

$$n(\varepsilon)d\varepsilon = \frac{g(\varepsilon)d\varepsilon}{\exp(-\lambda_1 + \varepsilon/k_B T) + 1}.$$

The total number of electrons is fixed and is given by integrating the normalisation condition:

$$N = \int_0^\infty \frac{g(\varepsilon)d\varepsilon}{\exp(-\lambda_1 + \varepsilon/k_B T) + 1}$$

In principle, we could solve for the Lagrange multiplier λ_1 . It is common practice to express it in terms of μ as follows:

$$\exp(-\lambda_1) = \exp(-\mu/k_B T)$$

μ is called the "chemical potential."

Occupying the energy states

For convenience, we define the following function:

$$f(\varepsilon) = \frac{n(\varepsilon)}{g(\varepsilon)} = \frac{1}{\exp((- \mu + \varepsilon)/k_B T) + 1}$$

Since $g(\varepsilon)d\varepsilon$ is the number of states and $n(\varepsilon)d\varepsilon$ is the number of particles, $f(\varepsilon)$ would be the fraction of states that are occupied.

So $f(\varepsilon)$ is called the occupation number. We need to get a feel as to what this looks like and how it changes with temperature.

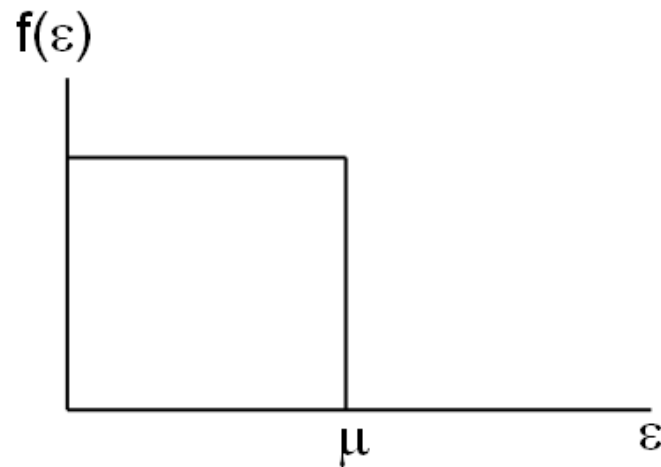
Lets start with the simplest case: $T = 0\text{K}$. If we allow T to approach zero, we will find:

$$\begin{aligned} f(\varepsilon) &= 1 \text{ for } \varepsilon < \mu \\ f(\varepsilon) &= 0 \text{ for } \varepsilon > \mu \end{aligned}$$

This means that all states with energy below μ are fully occupied. All states with energy above μ are empty.

Occupying the energy states

The graph for $f(\varepsilon)$ looks like this

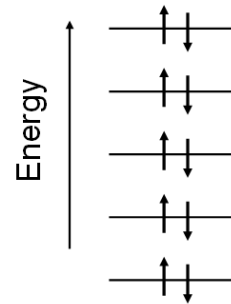


The shape shows that the energy levels are occupied below a certain energy, and unoccupied above that.

This feature is characteristic of the Fermi-Dirac distribution that we are studying.

The Fermi energy

At $T = 0\text{K}$, The highest energy in the stack of electrons is μ . This energy is also called the Fermi energy, E_F .



We can find the Fermi energy E_F by integrating the normalisation condition:

$$N = 2 \times \int_0^{\infty} n(\varepsilon) d\varepsilon$$

The factor of 2 must be added because each energy level can be occupied by 2 electrons - spin up and spin down.

We shall solve this for the Fermi energy E_F .

The Fermi energy

In terms of the occupation number,

$$n(\varepsilon) = g(\varepsilon)f(\varepsilon)$$

So the normalisation condition can be written as:

$$N = 2 \times \int_0^\infty n(\varepsilon)d\varepsilon = 2 \times \int_0^\infty g(\varepsilon)f(\varepsilon)d\varepsilon$$

We know that at 0K, $f(\varepsilon) = 0$ for $\varepsilon > \mu$. So the integration would stop at $\varepsilon = \mu$:

$$N = 2 \times \int_0^{E_F} g(\varepsilon)f(\varepsilon)d\varepsilon$$

since $\mu = E_F$ at 0K.

We also know that at 0K, $f(\varepsilon) = 1$ for $\varepsilon < \mu$. So

$$N = 2 \times \int_0^{E_F} g(\varepsilon)d\varepsilon$$

The Fermi energy

We have previously derived the density of states:

$$g(\varepsilon) = \frac{4m\pi V}{h^3} (2m\varepsilon)^{1/2}$$

In the topic on ideal gas, this is obtained by counting the number of energy states of a particle in a 3-D box. In this topic on electrons, we have used the same particle in a box. The difference from ideal gas only arises later on, when we make different assumptions about the energy levels.

So the same formula for the density of states can be used for both the ideal gas and the electrons. We can therefore substitute the formula into the normalisation integral

$$N = 2 \times \int_0^{E_F} g(\varepsilon) d\varepsilon$$

and solve for the Fermi energy. The result is

$$E_F = \frac{\hbar^2}{2m} \left(\frac{3\pi^2 N}{V} \right)^{2/3}.$$

Chemical potential

We have previously mentioned that the chemical potential in thermodynamics is the Gibbs free energy at equilibrium. E.g. it could be the heat change when 1 mole of vapour condenses:

$$\Delta\mu = \Delta U + p\Delta V - T\Delta S.$$

We have just seen that at 0 K, the chemical potential for an electron gas is the maximum energy of the electrons - the Fermi energy. We may think of this as the energy change if we remove 1 electron from the gas.

In both cases, the chemical potential is the energy change when the number of particles in a system is changed.

http://en.wikipedia.org/wiki/Chemical_potential

2.2 Electronic heat capacity

We want to use the ideas and formulae that we have developed to calculate the heat capacity of electrons.

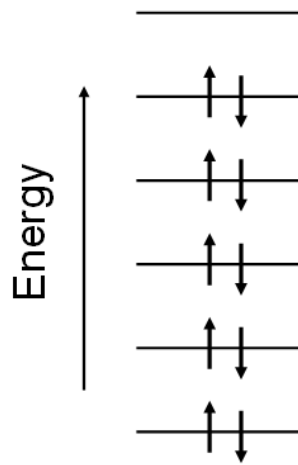
To see how to do this, recall that the Drude model would predict a heat capacity for that is the same as that of an ideal gas:

$$C = \frac{3}{2}Nk_B.$$

It is known from experiments that the actual heat capacity of the electrons is much smaller. This refers to measurements that are done at room temperature.

Heat capacity

We can understand this if we think that the electrons that are stacked up to the Fermi energy do not have enough energy to jump out of the stack.



This would only be true if the thermal energy is much smaller than the Fermi energy.

In order to find out if this is true, we need to estimate this thermal energy.

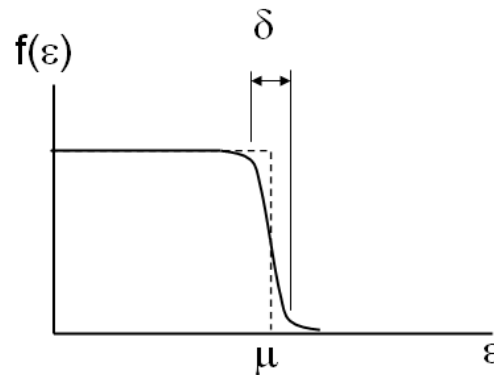
Heat capacity

We start by assuming that the thermal energy is indeed much smaller than the Fermi energy. We shall derive an expression for this thermal energy, and then calculate it at room temperature to see if the assumption can be justified.

At a temperature above 0 K, the occupation number

$$f(\varepsilon) = \frac{1}{\exp((- \mu + \varepsilon)/k_B T) + 1}$$

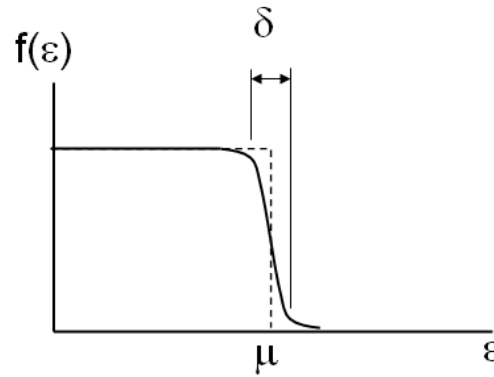
would no longer have a sharp step at the Fermi energy.



If $k_B T$ is much smaller than μ , the graph would remain close to the step, as if the step has become smoother.

Heat capacity

The "smoothened" slope of the graph tells us that electrons just below the Fermi energy ($\mu = E_F$) is excited just above it.



So we can estimate gain in thermal energy of the excited electrons by the width δ of this slope.

In order to do this, we take a closer look at the occupation number

$$f(\epsilon) = \frac{1}{\exp[(\epsilon - \mu)/k_B T] + 1}$$

Heat capacity

We are assuming that $k_B T$ is much smaller than μ .

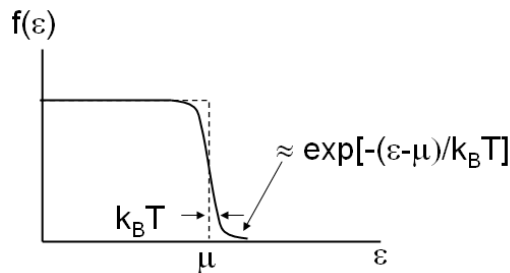
For energy ε higher than μ by a few times of $k_B T$, The exponential function $\exp[(\varepsilon - \mu)/k_B T]$ would quickly become large.

The occupation number is then approximately

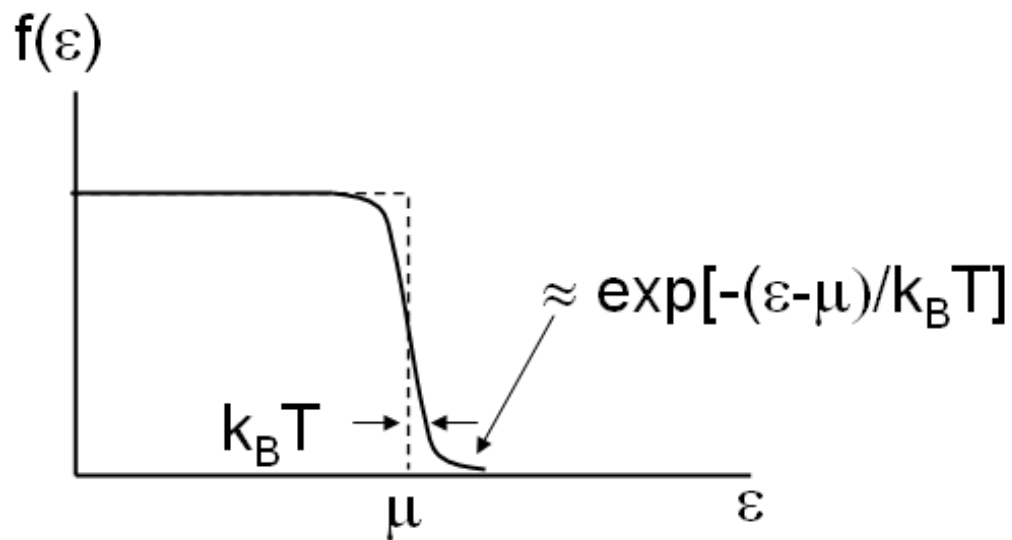
$$f(\varepsilon) = \frac{1}{\exp[(\varepsilon - \mu)/k_B T] + 1} \rightarrow \frac{1}{\exp[(\varepsilon - \mu)/k_B T]}$$

which is just the exponential function with negative argument

$$f(\varepsilon) = \exp[-(\varepsilon - \mu)/k_B T].$$



This means that the part of the graph to the right of μ falls off exponentially.



It falls by a fraction of $1/e$ over an energy range of $k_B T$.

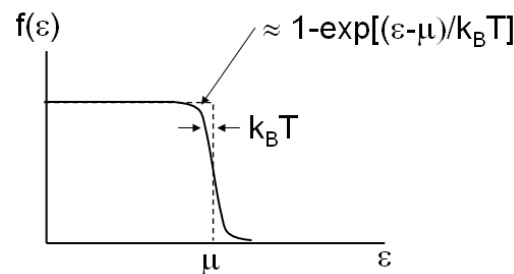
There is a corresponding behaviour just below the Fermi energy.

For energy ε lower than μ by a few times of $k_B T$, The exponential function $\exp[(\varepsilon - \mu)/k_B T]$ would quickly become small.

The occupation number is then approximately

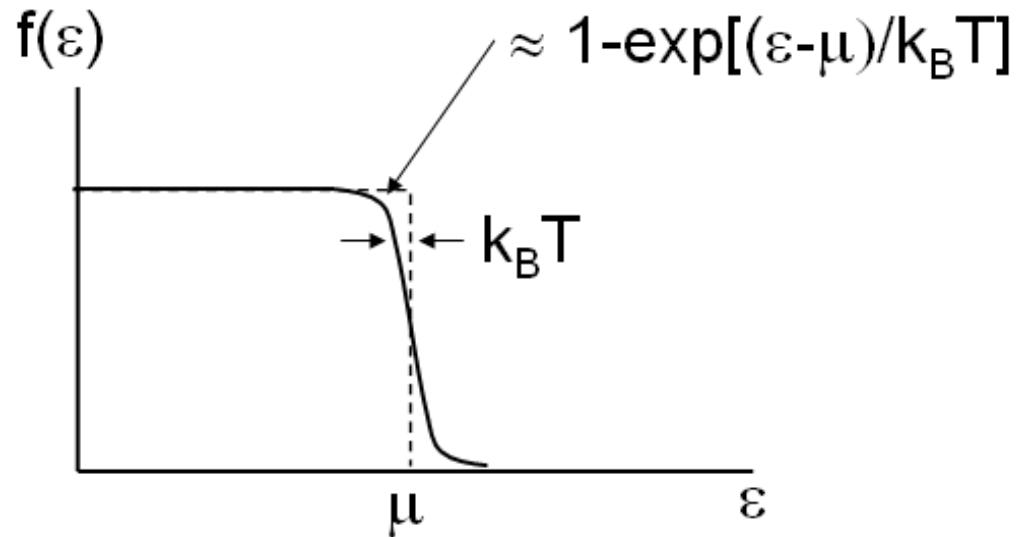
$$f(\varepsilon) = \frac{1}{\exp[(\varepsilon - \mu)/k_B T] + 1} \rightarrow 1 - \exp[(\varepsilon - \mu)/k_B T]$$

where we have used the binomial expansion and kept only the first order term.



Heat capacity

This means that the part of the graph to the left of μ tends to the line $f(\varepsilon) = 1$ exponentially.



It reaches within $f(\varepsilon) = 1$ by a fraction of $1/e$, over an energy range of $k_B T$.

This means that it is the electrons within this energy range that is excited. So the thermal energy of the excited electrons is of the order of $k_B T$.

At this point, we should justify our assumption that $k_B T$ at room temperature is much smaller than the Fermi energy $\mu = E_F$, which is defined at 0 K.

We shall take sodium metal as an example, and calculate $k_B T$ and E_F for this metal.

In sodium, each atom has one valence electron. This electron is mobile and forms the electron gas that we are talking about. In order to calculate the Fermi energy, we need the number density N/V . We can calculate this from the following data:

$$\text{density} = 0.97 \text{ g cm}^{-3}$$

$$\text{relative atomic mass} = 23.0$$

So the volume for one mole of atoms is

$$23 \div 0.97 = 23.71 \text{ cm}^3,$$

and the number density is

$$\frac{N}{V} = N_A \div 23.71$$

where N_A is Avogadro's number. This gives an answer of $2.54 \times 10^{28} \text{ m}^{-3}$.

Using the Fermi energy formula,

$$E_F = \frac{\hbar^2}{2m} \left(\frac{3\pi^2 N}{V} \right)^{2/3}.$$

where m is the mass of the electron, we can find that the Fermi energy is 3.16 eV.

In contrast, at room temperature 298 K, we can calculate that

$$k_B T \approx \frac{1}{40} \text{eV}.$$

This is about 120 times smaller than the Fermi energy.

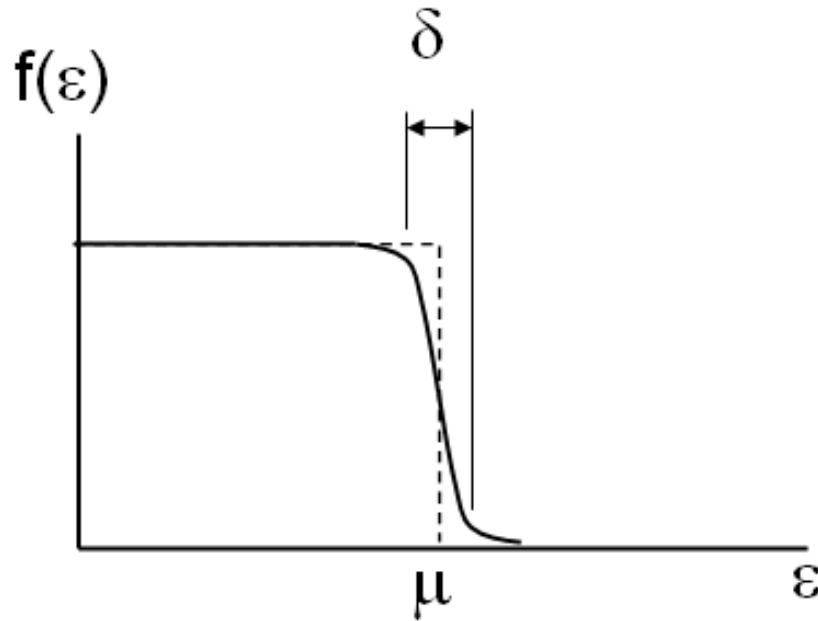
We can repeat this for other typical metals, and we would get similar answers.

This justifies our assumption that at room temperature $k_B T$ is much smaller than the Fermi energy.

We are now a step closer to estimating the electronic heat capacity. Next, we need to understand the behaviour of the excited electrons.

Heat capacity

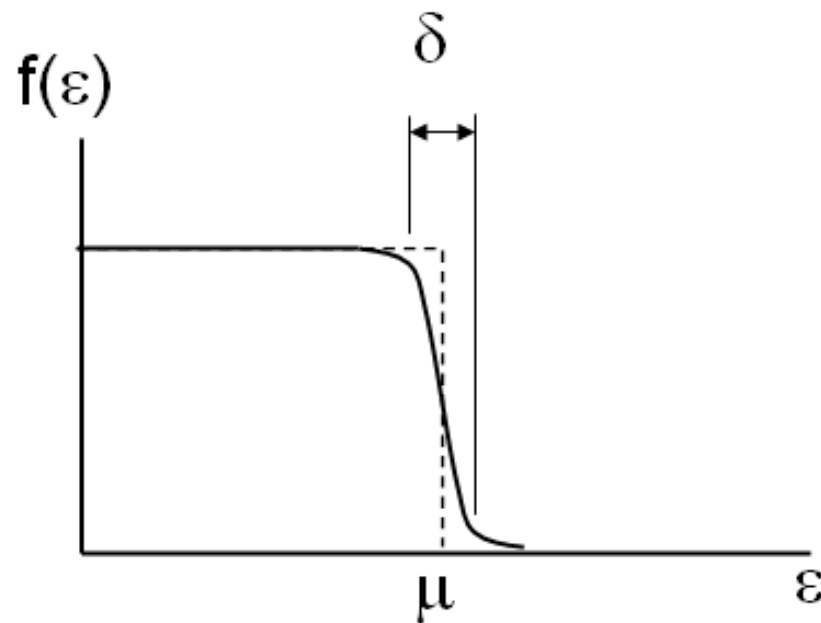
When temperature increases above 0 K, the step in the Fermi-Dirac distribution becomes smoother as electrons just below the Fermi energy are excited above it.



Notice that the "tail end" of the distribution - to the right - looks exponential. This is because there are relatively few electrons above the Fermi energy. So these can behave like the ideal gas and approximately obey the Maxwell-Boltzmann distribution.

Heat capacity

It is clear from the graph that for a small increase in temperature, only electrons close to the Fermi energy are excited. Most of the electrons are below the Fermi energy and are not excited at all. Since they cannot be excited, these electrons would not contribute to the heat capacity .



So it is mainly the electrons close to the Fermi energy that would contribute to the heat capacity. So we can use these to estimate the heat capacity and ignore the rest.

As we have seen, these electrons close to the Fermi energy behave like the ideal gas. We know that the energy of an ideal gas is

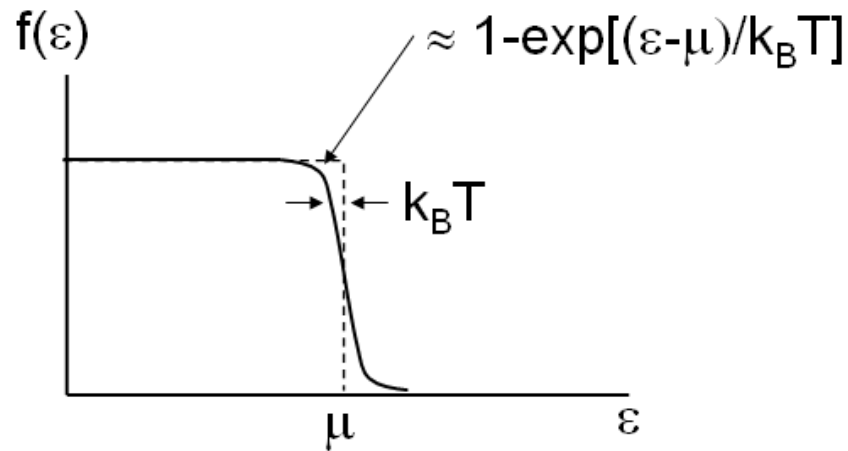
$$U_1 = \frac{3}{2}N_1k_BT$$

where N_1 is the number of particles in the ideal gas.

In the case of the electrons, N_1 should refer to the number of electrons above the Fermi energy, and not the total number of electrons. We can estimate this number as follows.

Heat capacity

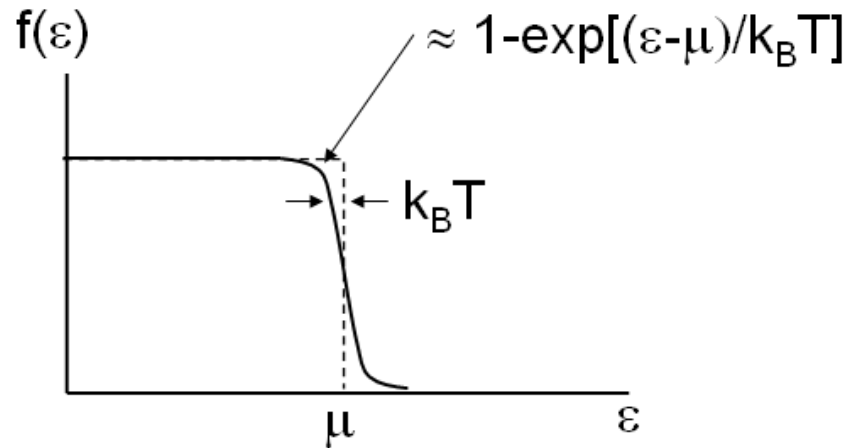
The electrons that do get excited are in the small energy range of order $k_B T$ from the Fermi energy E_F .



So we can estimate N_1 with the number of electrons that are within the energy interval of

$$d\epsilon = k_B T$$

from the Fermi energy.



We know that the number of particles in a given energy interval is

$$n(\epsilon)d\epsilon = 2g(\epsilon)f(\epsilon)d\epsilon$$

where the factor of 2 again comes from the spin states of the electrons.

At 0K, the energy states below E_F are fully occupied, i.e. $f(\epsilon) = 1$. So the number would given by

$$N_1 \approx 2g(E_F)k_B T$$

Heat capacity

From the definitions of the density of state and the Fermi energy, it can be shown (see exercises) that

$$g(E_F) = \frac{3N}{4E_F}$$

where N is the total number of electrons. This gives

$$N_1 \approx 2 \left(\frac{3N}{4E_F} \right) k_B T = \frac{3}{2} N \frac{k_B T}{E_F}$$

Substituting into the energy for ideal gas

$$U_1 = \frac{3}{2} N_1 k_B T$$

we get the energy for the excited electrons

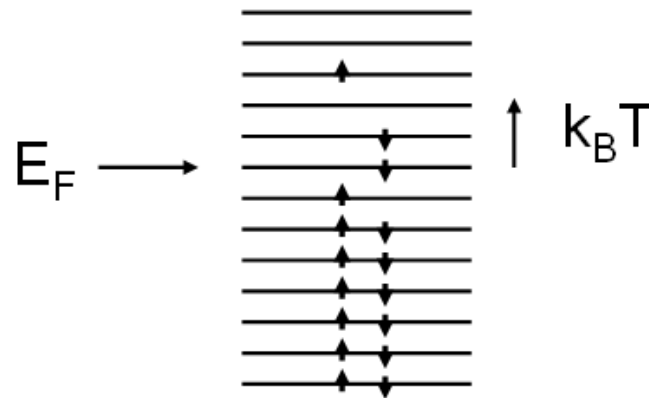
$$U_1 = \frac{3}{2} \left(\frac{3}{2} N \frac{k_B T}{E_F} \right) k_B T = \frac{9}{4} N k_B \frac{k_B T^2}{E_F}$$

Differentiating with respect to T , we get the electronic heat capacity

$$C = \frac{9}{2} N k_B \frac{k_B T}{E_F}$$

We summarise what we have learnt about the heat capacity:

Some states below Fermi level becomes empty, and some states above becomes occupied.



For a temperature T , an electron that gets excited would be able to gain on average an energy of about $3k_B T/2$.

Heat capacity

1. Only electrons within $k_B T$ of the Fermi level can jump up. Those further down cannot jump because the states above are still mostly occupied.

2. The number of electrons that can get excited is $\frac{3k_B T}{2E_F} N$. This is a fraction $\frac{3k_B T}{2E_F}$ of the total.

3. Each would gain an energy of about $3k_B T/2$. So the increase in total energy is obtained by multiplying the number of excited electrons by this energy

$$\Delta U \approx \frac{3k_B T}{2E_F} N \times 3k_B T/2 = \frac{9}{4} N k_B \frac{k_B T^2}{E_F}.$$

4. Differentiating with respect to T , we get the electronic heat capacity

$$C = \frac{9}{2} N k_B \frac{k_B T}{E_F}$$

We have obtained the electronic heat capacity

$$C = \frac{9}{2} N k_B \frac{k_B T}{E_F}$$

More detailed calculations show that the factor of $9/2$ should really be $\pi^2/2$:

$$C = \frac{\pi^2}{2} N k_B \frac{k_B T}{E_F}$$

This equation is often written in the form

$$C = \frac{\pi^2}{2} N k_B \frac{T}{T_F}$$

where $T_F = E_F/k_B$ is called the Fermi temperature.

Heat capacity of a metal

Notice that the heat capacity is directly proportional to T .

$$C = \frac{\pi^2}{2} N k_B \frac{T}{T_F}$$

This is often written in the form

$$C = \gamma T.$$

There is another contribution to the heat capacity. This comes from the vibrations of the atoms, and it is proportional to T^3 .

We could imagine writing the total heat capacity in the form:

$$c_V = \gamma T + AT^3.$$

We can measure this heat capacity to check if the formula is correct. Suppose that we have obtained a table of values for T and c_V . To check if the formula is correct, we can rewrite it in this form:

$$c_V/T = \gamma + AT^2$$

If we plot c_V/T against T^2 , we should get a straight line.

Heat capacity of a metal

In 1955, William Corak and his fellow co-workers measured the heat capacities of copper, gold and silver from 1K to 5K in their laboratory in Pittsburgh ...

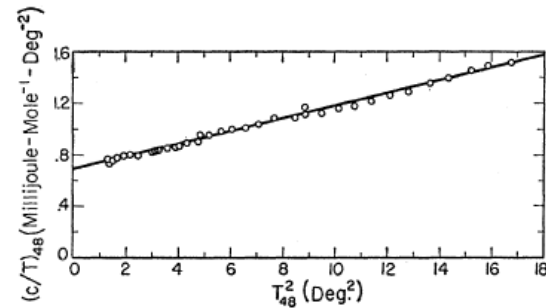
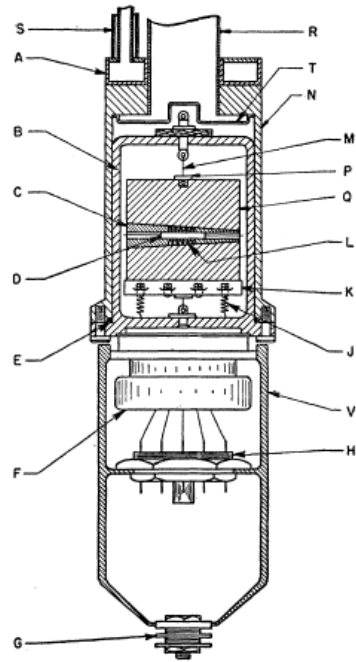


FIG. 5. Atomic heat of copper.

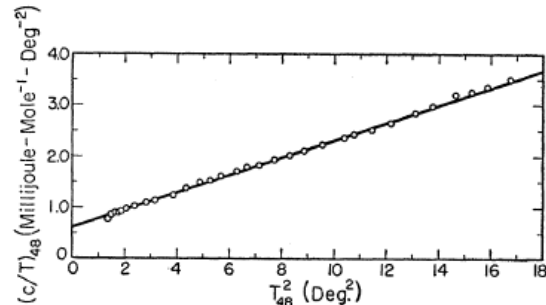


FIG. 6. Atomic heat of silver.

W. S. Corak, et al, Physical Review, vol. 98 (1955) pp. 1699-1707

and got the straight lines. This shows that the predictions of the Fermi-Dirac statistics are correct.

2.3 Effective mass, and a few other things

Heat capacity of a metal

From the formula,

$$c_V/T = \gamma + AT^2$$

we know that we can find γ from the y-intercept of the graph. The following table shows the values for a few metals.

ELEMENT	FREE ELECTRON γ (in 10^{-4} cal-mole $^{-1}$ -K $^{-2}$)	MEASURED γ	RATIO ^a (m^*/m)
Li	1.8	4.2	2.3
Na	2.6	3.5	1.3
K	4.0	4.7	1.2

The second column contains the values of γ from the formula:

$$C = \frac{\pi^2}{2} N k_B \frac{k_B T}{E_F} = \gamma T$$

The third column contains the values actually measured. They are obviously different.

Does this mean that our theory is wrong?

Yes and no. The theory tells us that the electronic heat capacity is proportional to T . The measurement shows that there is indeed such a contribution.

So we are not completely wrong. Perhaps the theory needs refining. We can be optimistic and go back and try and understand what we have missed.

Recall that we have started with a particle in a 3-D box and calculated the energy levels. Then we just fill these up with electrons and calculated the heat capacity. All we have is a gas of electrons in empty space.

But what about the atoms? The "empty space" is really filled with atoms. The electrons must surely interact with the atoms. This then is the reason for the difference between theory and measured γ .

However, the measured C is proportional to T . This agrees with theory, and it should mean something. One possibility is that, for some reason, the electron interacts only weakly with the atoms. This idea has been shown to be correct by other types of measurements.

According to this idea, the behaviour of the electrons in the presence of the atoms is essentially the same. The difference is that the interaction with the atoms make the electrons behave as if they have a different mass.

Heat capacity of a metal

If we imagine that the electrons in a metal has a different effective mass m^* than its natural mass, we can "explain" the difference in γ .

According to the formula for heat capacity, calculated γ is given by

$$\gamma = \frac{\pi^2}{2} N k_B \frac{k_B}{E_F}$$

This is inversely proportional to the Fermi energy

$$E_F = \frac{\hbar^2}{2m} \left(\frac{3\pi^2 N}{V} \right)^{2/3}.$$

which is in turn inversely proportional to the mass m of the electron.

So γ is directly proportional to the mass.

Heat capacity of a metal

This means that we can get the effective mass if we divide the measured γ (in the third column) by the calculated γ (in the second column).

This is shown in the last column of the table.

ELEMENT	FREE ELECTRON γ (in 10^{-4} cal-mole$^{-1}$-K$^{-2}$)	MEASURED γ	RATIO^a (m^*/m)
Li	1.8	4.2	2.3
Na	2.6	3.5	1.3
K	4.0	4.7	1.2

Behaviour at high temperatures

At very high temperatures, all the electrons could get excited. Then they would start to behave like an ideal gas. There are many more energy states they can reach and they are much less likely to be forced towards the same energy states.

This would happen only if the electrons are excited far above the Fermi energy. Therefore we can use Fermi temperature as a reference. A temperature would be high if it is high compared to the Fermi temperature.

At the high temperature, the heat capacity would therefore change to that of the ideal gas. So instead of

$$C = \frac{\pi^2}{2} N k_B \frac{T}{T_F}$$

which is very small, it would become

$$C = \frac{3}{2} N k_B$$

which is much larger.

A note on the chemical potential

We have seen many times that the chemical potential μ is equated to the Fermi energy E_F . It is important to note that this is true only at 0 K.

Recall the chemical potential μ is determined by the number of particles:

$$N = \int_0^\infty \frac{g(\varepsilon)d\varepsilon}{\exp[(\varepsilon - \mu)/k_B T] + 1}$$

At $T = 0$ K, the integral is just

$$N = \int_0^\mu g(\varepsilon)d\varepsilon$$

which is why μ is the Fermi energy then.

At higher temperature, μ would change. But for temperatures well below the Fermi temperature, as with electrons in metals at room temperature, we may assume that μ is still quite close to the Fermi energy.

Note that electrons belong to a larger family of particles called fermions.

A fermion is a particle with a half integer spin. Other examples are

- the proton,
- the neutron,
- the helium-3 (^3He) atom and
- the oxygen-13 (^{13}O) atom.

All fermions are known to show the kind of properties we have seen for electrons. They obey the Fermi-Dirac statistics.

What we have learnt so far

1. Electrons follow the Fermi-Dirac distribution:

$$n(\varepsilon)d\varepsilon = \frac{g(\varepsilon)d\varepsilon}{\exp[(\varepsilon - \mu)/k_B T] + 1}.$$

2. At 0 K, the electrons fill up the energy states from the lowest level. The highest energy of the electrons is called the Fermi energy:

$$E_F = \frac{\hbar^2}{2m} \left(\frac{3\pi^2 N}{V} \right)^{2/3}.$$

3. When thermal energy $k_B T$ is small compared to the Fermi energy, only electrons near the Fermi energy would get excited. So only these would contribute to the electronic heat capacity:

$$C = \frac{\pi^2}{2} N k_B \frac{T}{T_F}$$

4. The Fermi temperature is defined as

$$T_F = \frac{E_F}{k_B}$$

2.4 Exercises

Exercise 1

Show that the density of states at the Fermi energy E_F is given by

$$g(E_F) = \frac{3N}{4E_F}$$

where N is the number of electrons.

Exercises

We can make use of the following relations for the density of states.

Relation with the total number of states:

$$g(\varepsilon) = \frac{G(\varepsilon)}{d\varepsilon}.$$

Formula for the total number of states:

$$G(\varepsilon) = \frac{4\pi V}{3h^3} (2m\varepsilon)^{3/2}$$

so

$$G(\varepsilon) \propto \varepsilon^{3/2}.$$

Relation with the Fermi energy and N :

$$N = 2 \int_0^{E_F} g(\varepsilon) d\varepsilon.$$

Exercises

From

$$g(\varepsilon) = \frac{G(\varepsilon)}{d\varepsilon}$$

and

$$N = 2 \int_0^{E_F} g(\varepsilon) d\varepsilon,$$

we have

$$N = 2G(E_F).$$

From

$$G(\varepsilon) \propto \varepsilon^{3/2},$$

we have

$$\frac{g(\varepsilon)}{G(\varepsilon)} = \frac{3}{2\varepsilon}.$$

At the Fermi energy E_F , we get ...

$$g(E_F) = \frac{3G(E_F)}{2E_F}.$$

Substituting the above result for N :

$$N = 2G(E_F),$$

we get

$$g(E_F) = \frac{3N}{4E_F}.$$

Exercise 2

The number of ways of arranging fermions is given by

$$\Omega = \prod_i \frac{g_i!}{n_i!(g_i - n_i)!}.$$

Use this formula, along with the conservation of particle number and total energy, to derive the Fermi-Dirac distribution function:

$$\frac{n_i}{g_i} = \frac{1}{\exp(-\lambda_1 - \lambda_2 \varepsilon_i) + 1}$$

where λ_1 and λ_2 are the Lagrange multipliers.

Exercises

We need to maximise the Lagrange function $\ln \Omega + \lambda_1 N + \lambda_2 U$.

Using Stirling's formula

$$\ln N! \approx N \ln N - N$$

we have

$$\ln \Omega \approx \sum_i g_i \ln g_i - g_i - (n_i \ln n_i - n_i) - [(g_i - n_i) \ln(g_i - n_i) - (g_i - n_i)]$$

Differentiating with respect to n_i ,

$$\frac{\partial \ln \Omega}{\partial n_i} = -\ln n_i + \ln(g_i - n_i) = \ln \frac{g_i - n_i}{n_i}$$

The total number is given by

$$N = \sum_i n_i,$$

and the total energy by

$$U = \sum_i n_i \varepsilon_i.$$

Differentiating these ...

Exercises

We get

$$\frac{\partial \ln N}{\partial n_i} = 1$$

and

$$\frac{\partial \ln U}{\partial n_i} = \varepsilon_i.$$

Then differentiating the Lagrange function, we get

$$\ln \left(\frac{g_i - n_i}{n_i} \right) + \lambda_1 + \lambda_2 \varepsilon_i = 0$$

Rearranging, we get the Fermi-Dirac distribution function:

$$\frac{n_i}{g_i} = \frac{1}{\exp(-\lambda_1 - \lambda_2 \varepsilon_i) + 1}.$$

Exercise 3

Show that the mean energy of electrons at absolute zero, $\bar{\epsilon}$ is $3E_F/5$, where E_F is the Fermi energy.

Exercises

The total energy is

$$U = \int_0^{\infty} n(\varepsilon) \varepsilon d\varepsilon.$$

For the Fermi-Dirac distribution,

$$U = 2 \int_0^{\infty} g(\varepsilon) f(\varepsilon) \varepsilon d\varepsilon.$$

At 0 K, this would be

$$U = 2 \int_0^{E_F} g(\varepsilon) \varepsilon d\varepsilon.$$

Recall the density of states

$$g(\varepsilon) = \frac{4m\pi V}{h^3} (2m\varepsilon)^{1/2}.$$

Substituting into the integral,

$$U = 2 \int_0^{E_F} \frac{4m\pi V}{h^3} (2m\varepsilon)^{3/2} d\varepsilon.$$

Exercises

Integrating,

$$U = 2 \frac{4m\pi V}{h^3} (2m)^{3/2} \frac{2}{5} E_F^{5/2}$$

To relate this to N ,

$$N = 2 \int_0^{E_F} g(\varepsilon) d\varepsilon.$$

we substitute the density of states

$$N = 2 \int_0^{E_F} \frac{4m\pi V}{h^3} (2m\varepsilon)^{1/2} d\varepsilon$$

and integrate:

$$N = 2 \frac{4m\pi V}{h^3} (2m)^{3/2} \frac{2}{3} E_F^{3/2}$$

The average energy is the energy per particle

$$\bar{\varepsilon} = \frac{U}{N} = \frac{3}{5} E_F$$

Exercise 4

Metallic hydrogen can be produced by compressing liquid hydrogen to extremely high pressure. This transition has been observed when the density reaches $0.32 \times 10^6 \text{ mole m}^{-3}$, at a temperature of 3000 K. It is thought that in the metallic phase the liquid comprises H_2^+ ions and electrons. Were the electrons in this liquid metal obeying classical or Fermi-Dirac statistics.

Exercises

We need to compare the 3000 K temperature to the Fermi temperature T_F .

If the temperature is much higher than T_F , the electrons would obey classical statistics and behave as an ideal gas. If the temperature is much smaller than T_F , the electrons would obey Fermi-Dirac statistics.

The Fermi temperature is related to the Fermi energy by

$$T_F = \frac{E_F}{k_B}$$

and the Fermi energy is given by

$$E_F = \frac{\hbar^2}{2m} \left(\frac{3\pi^2 N}{V} \right)^{2/3}.$$

where m is the mass of the electron.

Exercises

The hydrogen density $0.32 \times 10^6 \text{ mole m}^{-3}$ is also the electron density, since each molecule H_2 converted to H_2^+ gives one electron. The number density is obtained by multiplying Avogadro's constant:

$$\frac{N}{V} = (0.32 \times 10^6) \times (6.022 \times 10^{23}).$$

Substituting this and the other constants into the above formulae, we get the Fermi temperature

$$T_F = 141,000K.$$

The temperature of 3000 K is therefore much lower than the Fermi temperature. So the electrons in metallic hydrogen would obey Fermi-Dirac statistics, in the same way as normal metals at room temperature.

Exercise 5

One possible means of obtaining fusion energy is to implode spherical capsules containing heavy hydrogen by irradiating them with high power lasers. For fusion to occur the implosion core needs to reach electron temperatures of the order of ~ 1 eV, and the electron density needs to be of the order of 10^{33} m^{-3} . Do we need to use Fermi-Dirac statistics to describe the electrons, or are Maxwell-Boltzmann statistics sufficient?

Exercises

We need to compare the 1 eV electron temperature to the Fermi energy E_F . The Fermi energy is given by

$$E_F = \frac{\hbar^2}{2m} \left(\frac{3\pi^2 N}{V} \right)^{2/3}.$$

The number density N/V is 10^{33} m^{-3} . Substituting into the above formula, we get

$$E_F = 3650 \text{ eV}.$$

The electron temperature of 1 eV is much smaller than this.

Therefore the electrons would be described by Fermi-Dirac statistics. They would behave like electrons in metal at room temperature, and not as an ideal gas.

Note

Notice that the terms energy and temperature have been used interchangeably.

A temperature of $E = 1$ eV, means that the temperature would be

$$T = E/k_B$$

in Kelvin.